Extension of NHWAVE to Couple LAMMPS for Modeling Wave Interactions with Arctic Ice Floes

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LONG-TERM GOALS

1. Developing and testing a tightly-coupled wave-ice model system, including a nonhydrostatic wave model (NHWAVE, Ma et al., 2012) and a discrete element model (LAMMPS/LIGGGHTS; Plimpton, 1995), for simulating wave interactions with arctic ice floes.
2. Using the coupled NHWAVE and LAMMPS/LIGGGHTS models to investigate the relative importance of key physical processes governing the attenuation of wave energy in the marginal ice zone (MIZ).
3. Conducting comparative simulations to evaluate MIZ dissipation parameterizations used by larger-scale ice-ocean models.

OBJECTIVES

The study is a collaborative effort with Mark Orzech, Jay Veeramony and Joe Calantoni of the Naval Research Laboratory (separate internal NRL project, funded for FY14-17). The objectives of this study are to

1. extend NHWAVE to incorporate wave interactions with moving obstacles.
2. collaborate with the NRL LAMMPS/LIGGGHTS group to develop matching boundary conditions for both NHWAVE and LAMMPS/LIGGGHTS in a two-way coupling system.
3. collaborate with the NRL LAMPPS/LIGGGHTS group to conduct a numerical study on determining the relative importance of key physical processes governing the attenuation of wave energy in the MIZ.

APPROACH

We have developed additional capabilities in NHWAVE so that it can be tightly coupled to LAMMPS/LIGGGHTS for use in modeling wave interactions with ice floes. This effort entails completion of the following approaches:

1. Implementation of 3D moving masks to represent ice floes in the computational image domain. A generalized vertical coordinate transformation is needed to make curvilinear coordinates fitting the ice floe boundaries.
2. Development of matching boundary conditions for coupling with LAMMPS/LIGGGHTS. Both the kinematic and dynamic boundary conditions are developed. Specifically the kinematic boundary conditions are applied using the numerical fluxes defined at the fluid-ice interface. The dynamic boundary conditions include the pressure gradient boundary condition at the moving object boundaries, the wave-ice shear stress, and the form drag. The immersed boundary (IB, e.g., Udaykumar et al., 1999) method is applied at the fluid-ice interface in the horizontal directions.
3. Enhancement of modularized NHWAVE to facilitate coupling interface development. The model architecture of NHWAVE is modified using object-oriented modularization techniques. To improve the model efficiency for modeling in an O(10km) scale domain, the Poisson pressure solver is enhanced using the Pressure Decimation and Interpolation Method (Shi et al., 2015).
4. Coordination with the LAMMPS/LIGGGHTS model group in NRL to test the coupled model. The work is a collaborative effort with the researchers of NRL, who focus on the mechanisms of wave-ice floe interaction using the coupled model and try to gain a better understanding of the relative importance of the major wave attenuation processes in the MIZ. We are focused on the development and testing of the coupled model and will assist the NRL group to carry out the process-based study.

WORK COMPLETED

In FY14, we focused on the extention of NHWAVE to include capabilities of modeling wave interaction with 3D moving objects. The work also includes implementations of efficient numerical schemes and boundary conditions for applications of wave-ice floe interaction in a large computational domain.

1. NHWAVE has been extended to a generalized vertical coordinate system by using a generalized sigma-coordinate transformation. This extension allows the model to apply the natural kinematic boundary conditions at the bottom and top surfaces of the ice floe. The generalized vertical coordinate is not limited to analytical expressions of the traditional sigma-coordinate used in most ocean models. It is flexible and can fit complex top and bottom surfaces of ice floes. The existing 2D mask in NHWAVE is extended to 3D, which can easily handle the movement and rotation of obstacles with the inclusion of mass conservation.

2. Formulations are implemented to compute kinematic and dynamic boundary conditions. Since the time-dependent boundary-fitted coordinate is applied at the top and bottom surfaces of an object, the kinematic boundary condition is naturally satisfied in the vertical direction at the

fluid-object interfaces. In the horizontal directions, the immersed boundary method is used for dynamic boundary conditions.

3. We developed a so-called Pressure Decimation and Interpolation method (PDI, Shi et al., 2015) for futher improvement of computational efficiency. Recent studies using Poisson solver-based non-hydrostatic models have shown that an accurate prediction of wave dispersion does not require a large number of vertical layers if the dynamic pressure is properly discretized. We have explored the possibility that the solution for the dynamic pressure field may, in general, be decimated to a resolution far coarser than used in representing velocities and other transported quantities, without sacrificing accuracy of solutions. In the new code, we determine the dynamic pressure field by solving the Poisson equation on a coarser grid and then interpolate the pressure field onto the finer grid used for solving the remaining dynamic variables. Computational efficiency of the model is greatly improved.

In FY 15, we carried out extensive model validations, development of model coupling framework, and tests of the coupled NHWAVE-LIGGGHTS model.

1. We have performed four basic tests of the wave interaction with floating objects, including wave reflectoin and transmission by a fixed floating object, wave radiation from a floating object heaving, swaying, and rolling. Model results agree very well with analytical solutions.
2. A laboratory experiment of waves generated by a bouncing ball was conducted at NRL, Stennis Space Center, in July and August, 2014. The measured wave data was used to validate the numerical model.
3. We collaborated with the NRL LAMMPS/LIGGGHTS group to develop the interface for coupling NHWAVE with LIGGGHTS which is an improved version of LAMMPS. Preliminary coupling tests show that the coupled model is well scaled in the DOD HPC system and capable of simulating wave-ice floe interaction in a large computational domain

RESULTS

The model with the newly developed capabilities of modeling wave-floating object interaction has been validated by comparison with analytical solutions for a 2D floating box and with a laboratory measurement of wave generation by a vertical oscillating sphere.

Figure 1 shows model comparisons with analytical solutions in tests of wave reflection and transmission by a fixed floating object (a), wave radiation from a floating object heaving (b), swaying (c) and rolling (d). The floating object is configured as a rectangular shape with a length of $2a$and, a draft of d, in water of depth h. In the test of wave reflection and transmission, the model predicts transmission rates decreasing with increasing khvalues, which agrees very well with analytical solutions. Satisfactory results are also obtained in cases of wave radiation from a moving object (rest of panels) in comparison to the analytical solutions for all khvalues.

Measured data from the laboratory experiment of waves generated by a bouncing ball was used to validate the model. Figure 2 shows modeled surface elevations at different locations in comparison to the measured data. Time series of the ball centroid is described in the top panel of

the figure. Time series of water surface at r = 0.45, 0.65, 0.85 and 1.05 m, where r is the distance from the center of the domain, are shown in the rest of the panels. The data points (crosses) are sparse due to the low scan frequency of the Lidar used in the experiement and are fitted by the dashed lines to better demonstrate the surface wave process at certain locations. The solid lines represent modeled surface elevations at the corresponding locations. The model/data comparison shows that the model is accurate in predicting waves generated by a prescribed moving object at the water surface, indicating its capability to model wave-surface object interactions when provided with realistic object motions by the coupled discrete element model.

The model coupling framework has been developed in the collaborative effort with the NRL group. Extensive tests of the coupled system have been performed in the DOD HPC system. Figure 3 demonstrates a test of wave-ice floe interation modeled by the coupled NHWAVE-LIGGGHTS system. The lower portions of the panels show snapshots of wave surface modeled by NHWAVE and ice floes (white cubes) modeled by LIGGGHTS at different times: (a) t=47.20s, (b) t=48.01s, (c) t=48.41s and (d) t= 52.01s. The upper portion of each panel shows the energy variation due to presence of ice floes, which is calculated by subtracting the flow energy (potential energy + kinetic energy) modeled with ice floes from the energy without ice floes. Tests with various configurations also indicate both NHWAVE and LIGGGHTS are well scaled in the large-scale parallel system.

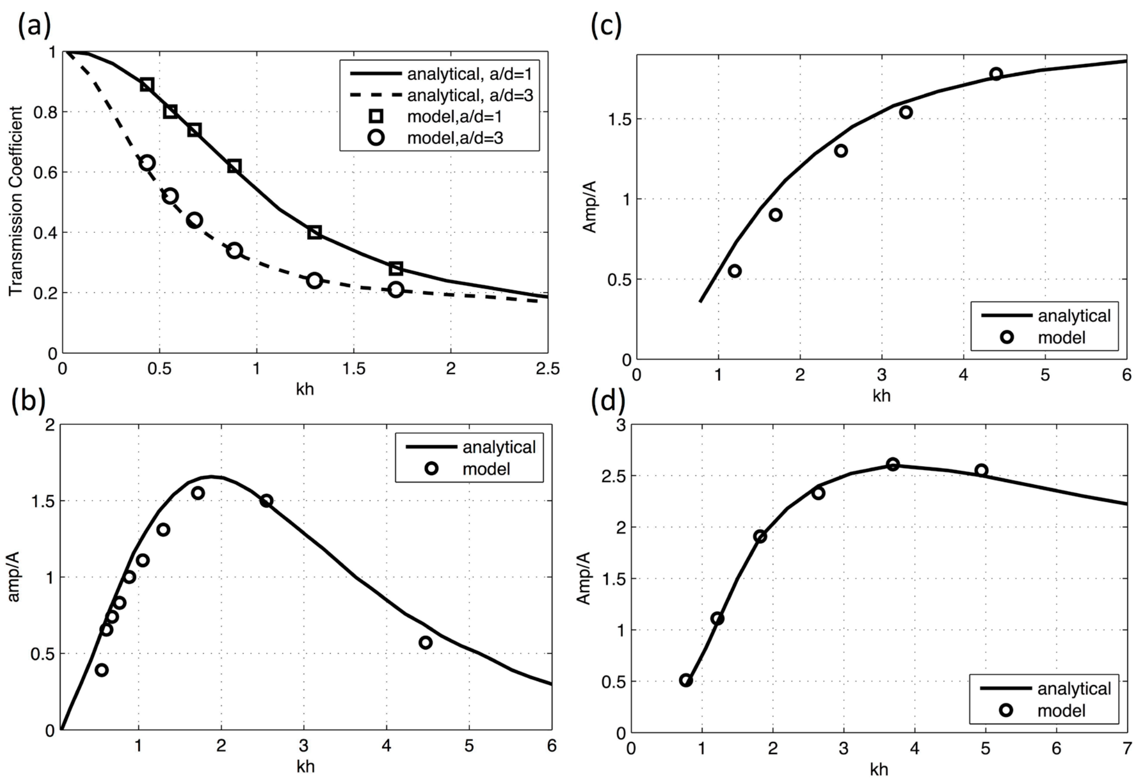

Figure 1. Comparisons between model results and analytical solutions. (a): wave transmission coefficient in the case of waves passing a floating rectangular object. (b)-(d): normalized amplitude of waves generated by floating object heaving (b), swaying (c), and rolling (d).

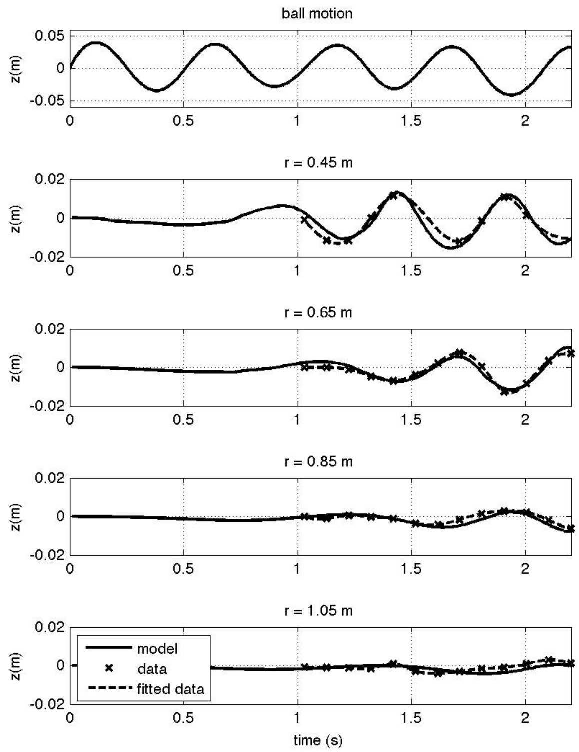

Figure 2. Comparison of surface elevation between model and experiment data (crosses: data, dashed lines: data fitted lines, solid lines: model results). The top panel shows the time series of the ball centroid location.

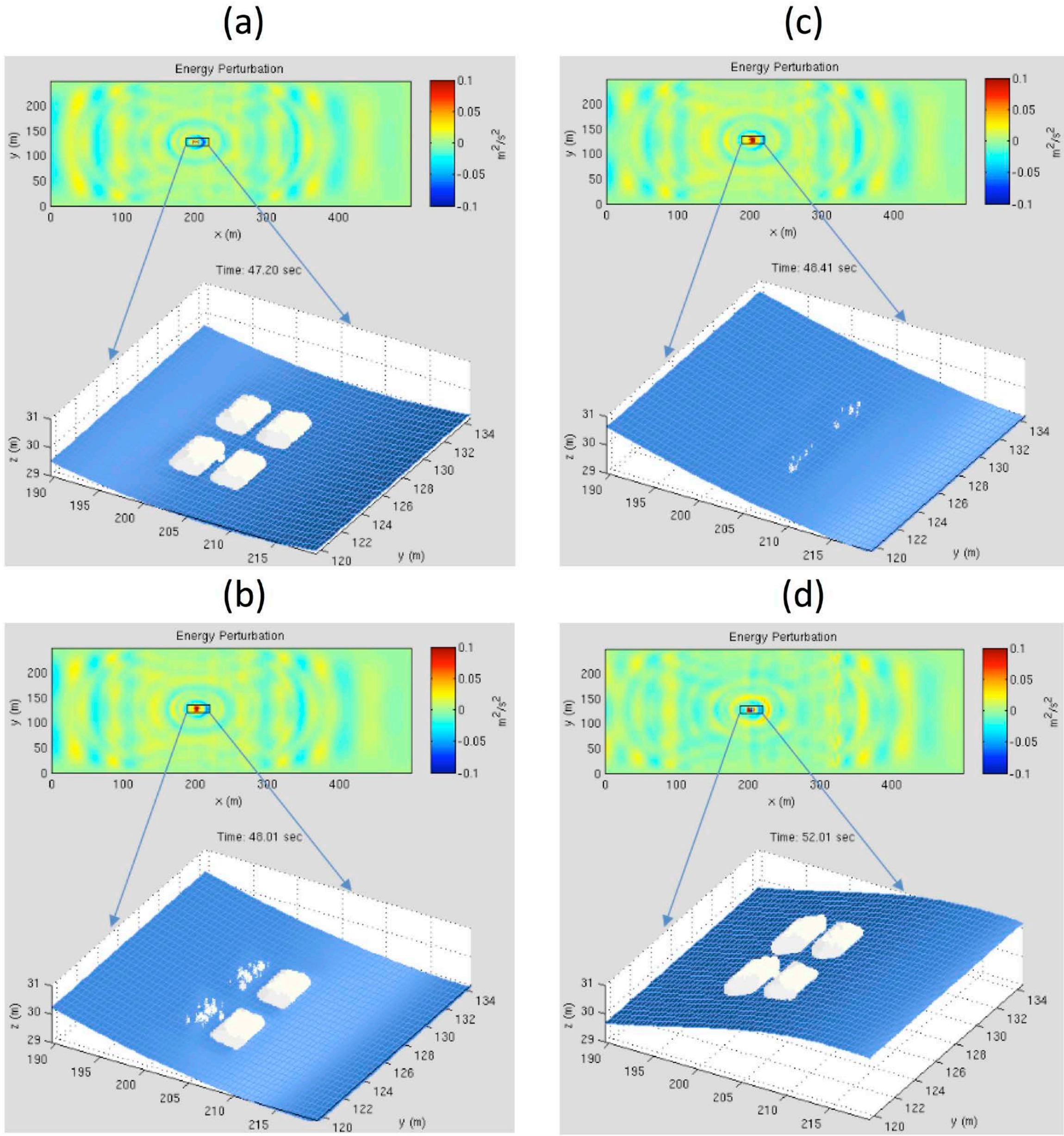

Figure 3. Test of coupling between NHWAVE and LIGGGHTS. Snapshots of wave surface modeled by NHWAVE and ice floes (white cubes) modeled by LIGGGHTS at different times: (a) t=47.20s, (b) t=48.01s, (c) t=48.41s and (d) t= 52.01s. The upper portion of each panel shows the energy variation due to presence of ice floes, which is calculated by subtracting the flow energy (potential energy + kinetic energy) modeled with ice floes from the energy without ice floes.

IMPACT/APPLICATIONS

Further development of NHWAVE is also supported by the ONR Littoral Geosciences and Optics Program, RIVET II project (N00014-13-1-0188; PIs: Hsu, Shi and Kirby), a NSF project (OCE-1334325; PIs: Kirby, Hsu, Shi and Ma), and a NSF project (OCE-1435147, PIs: Kirby and

Shi). The modularization of NHWAVE developed in the current project provides an important approach to enhancing the model efficiency for large-scale simulations.

RELATED PROJECTS

1. ONR RIVET II project. One of the main objectives is enhancement of NHWAVE with a high computational efficiency in order to carry out system-scale simulation with high resolution in the river plume nearfield.
2. NSF project (*OCE-1334325; Collaborative Research: The interaction of waves, tidal currents and river outflows and their effects on the delivery and resuspension of sediments in the near field; collaborate with Dr. Gangfang Ma of ODU*). The ongoing project is to study broader issues of wave-current interaction and sediment delivery in the nearfield of tidally-pulsed river plumes. NHWAVE is being extended to include more model components and boundary conditions such as the wave-current aborbing-generating condition which can be used in modeling wave-ice floe interaction under strong current conditions.

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